NA-ASC-500-07 Issue 7

June 2008

The Year So Far...

Editorial by Bob Meisner

The first half of this year has been one of significant success for the program in spite of the budget turmoil, achieved through the staunch determination of a world-class team spread across the labs. Your accomplishments continue to improve the way science and engineering are conducted, and I'd like to take this opportunity to recognize a few significant steps forward.

Congratulations to LANL for being the first on the planet to bring a general-purpose petaFLOPS machine to life. It is impossible to capture the magnitude of the challenges presented to the Roadrunner team and the lab in pulling this off. Suffice it to say that under extreme time, technical, and programmatic pressures, they did what many thought could not be done.

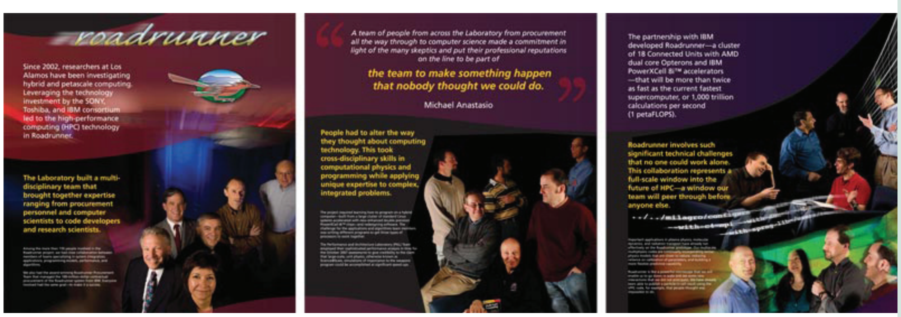
Though less flashy than a headline-grabbing supercomputer, the Tri-lab Linux Capacity Cluster procurement had its own set of unique complexities that made its achievement exemplary. What makes it stand out is the leadership and dedication of the team in building a cost-effective, tri-lab solution for the greater good of the program. As a result, for the first time since the dawn of ASCI, the labs will have a significant dedicated computational resource applied to the full spectrum of the production workload.

March saw the initiation of the New Mexico Alliance for Computing at Extreme Scale, or ACES. This is the second center formed through a collaboration by Sandia and Los Alamos, the first being the Center for Integrated Nanotechnologies. Born of the need to investigate innovation in high-end computing systems using cost-effective solutions, ACES is an icon that represents an entry point into the labs for academia and industry working with the ASC program at the New Mexico labs.

These accomplishments bring new excitement to the program because of their potential for advancing science and engineering on our way to predictive capabilities, not only for our stewardship mission, but also for other national needs. Congratulations to the hundreds of professionals that contributed to these successes. You make us all proud to be on the ASC team—nobody does it better.

Roadrunner Fastest Computer on Earth

On May 26, 2008, the Roadrunner supercomputer achieved the long-sought supercomputing goal of performing more than a thousand trillion operations per second, or petaFLOPS. Roadrunner was built by IBM with funding from the NNSA for Los Alamos National Laboratory. Soon, a caravan of moving vans will transport Roadrunner from IBM to Los Alamos, where it will be installed in the Nicholas C. Metropolis Center for Modeling and Simulation.



Shown here is a small cross section of people who collaborated across many sectors of Los Alamos National Laboratory to make Roadrunner a success. Roadrunner is an example of a project that is such a significant technical challenge that no one person could do it alone.

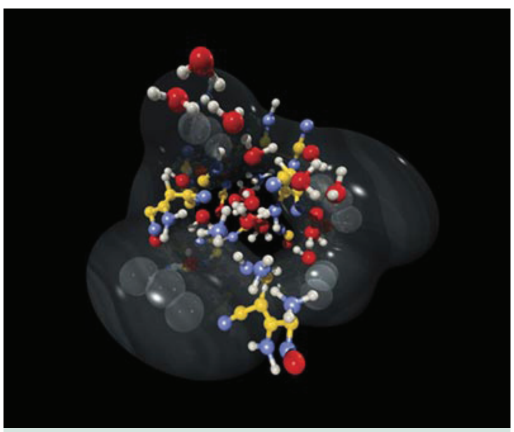
Roadrunner is a "hybrid supercomputer," integrating a new cell-based processor, designed and built by IBM with a traditional microprocessor supplied by AMD. Coupled with programs designed to utilize its unprecedented performance, Roadrunner will foster scientific discovery in many fields, ranging from physical sciences to biology and medicine, and it will provide a petaFLOPS-scale scientific computing capability for the nation's weapons program. Roadrunner is also rated as very energy efficient, using approximately the same total power as the recently retired Q system, with more than fifty times the performance.

Breaking the petaFLOPS barrier is a major milestone in the supercomputing world. According to Dr. Andrew White, Roadrunner project director at Los Alamos, "This is a remarkable achievement. The science will be even more so."

NNSA Creates an Alliance to Pursue Computing at Extreme Scales

NNSA's Advanced Simulation & Computing (ASC) program has established a high-performance capability computing partnership known as the NNSA Alliance for Computing at Extreme Scale (ACES). ACES is a joint venture between two New Mexico laboratories: Sandia National Laboratories and Los Alamos National Laboratory. As part of the Alliance, both laboratories will share intellectual capabilities and capitalize on their existing expertise in developing architectures and designs for future platforms. Los Alamos's Strategic Computing Complex (SCC) facility will house high-performance capability computing assets needed to support NNSA's ongoing stockpile stewardship mission, and to meet the ASC Roadmap timeline requirement for an exascale capability by 2018. The first of these ACES capability platforms will be named Zia and is targeted for installment in FY10. It will support the needs of all three NNSA's laboratories.

Explosives at the Microscopic Scale Produce Shocking Results



Simulations show that molecules in detonating high explosives take on metallic properties. Metallic molecules are translucent, while insulating molecules are colored according to atom type: hydrogen is white, carbon is yellow, nitrogen is blue, and oxygen is red.

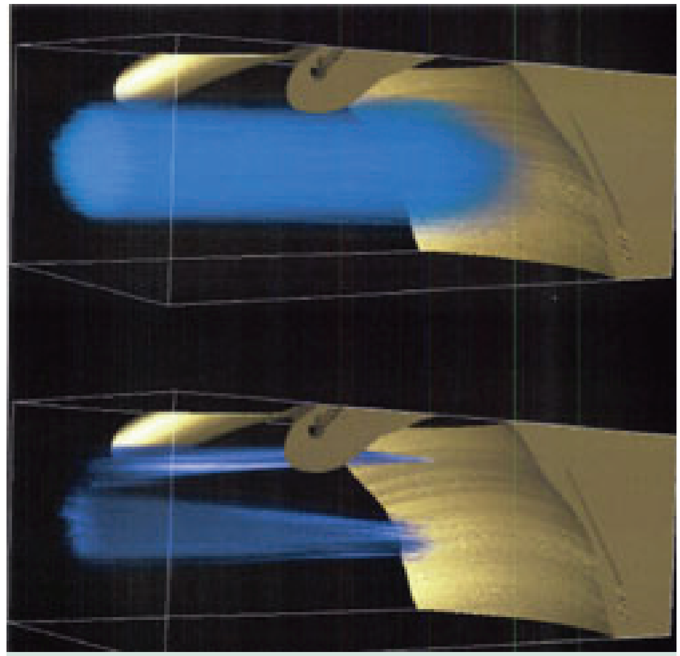
The first quantum molecular dynamics simulation of a shocked explosive near detonation conditions to reveal what happens at the microscopic scale was recently announced by researchers from Lawrence Livermore National Laboratory and the Massachusetts Institute of Technology. What they found was quite riveting: the explosive, nitromethane, undergoes a chemical decomposition and a transformation into a semi-metallic state for a limited distance behind the detonation front. "Despite the extensive production and use of explosives for more than a century, their basic microscopic properties during detonation haven't been unraveled," said lead author Evan Reed in a January 2008 article in Nature Physics. "We've gotten the first glimpse of the properties by performing the first quantum molecular dynamics simulation."

Nitromethane is burned as a fuel in drag racers but can also be made to detonate, a special kind of burning in which the material undergoes a much faster and far more violent type of chemical transformation. With its single NO_2 group, it is a simple, representative version of explosives with more NO_2 groups. Though it is an optically transparent, electrically insulating material, it turns into an optically reflecting, nearly metallic state for a short time behind the detonation shock wave front. Behind the wave front, the material returns to being optically transparent and electrically insulating. "This is the first observation of this behavior in a molecular dynamics simulation of a shocked material," Reed noted. "Ultimately, we may be able to create computer simulations of detonation properties of new, yet-to-be synthesized designer explosives."

Other Livermore researchers include M. Riad Manaa, Laurence Fried, Kurt Glaesemann, and J.D. Joannopoulos of MIT.

NIF Full-Beam Simulation on BlueGene/L a Success

Lawrence Livermore National Laboratory recently completed a parallel F3D (pF3D) simulation of a National Ignition Facility (NIF) 50-degree laser beam on the BlueGene/L computer. This is the first time that a simulation has modeled the full cross section of a NIF beam from the laser entrance hole to the hohlraum wall. Until now, simulating the entire beam cross section was beyond the reach of available computational resources. The BlueGene/L full-beam simulation provides a benchmark for evaluating the effects of approximating the beam by a central slab.



The incident laser simulates Brillouin scatter from two distinct regions.

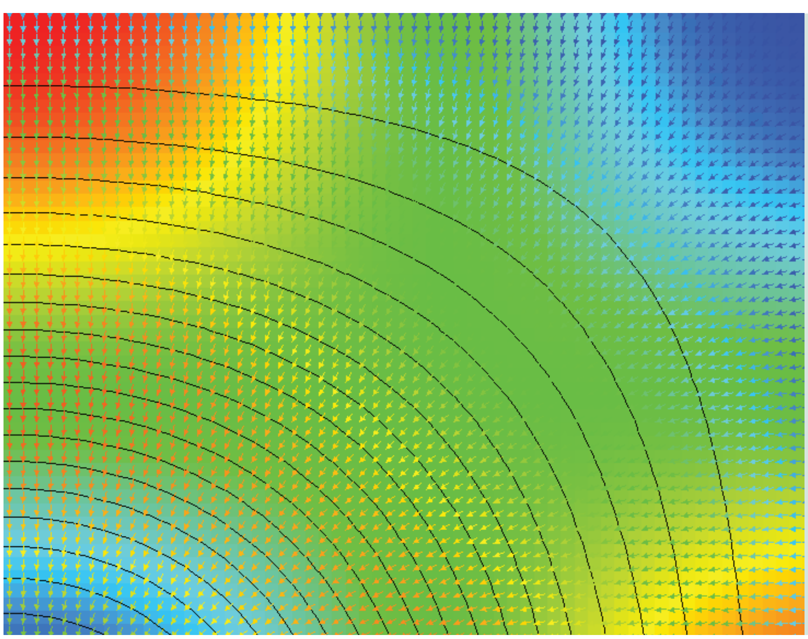
The simulation ran for about 10 days and 13 hours on 196,608 processors with approximately 24 billion zones, and pF3D demonstrated nearly ideal performance scaling on this massively parallel calculation. "This appears to be the highest processor count ever employed in a multiphysics simulation, and the results are being submitted for consideration for the 2008 Gordon Bell Prize," said LLNL Physicist Steve Langer. "Most Gordon Bell winners in the past have had a single compute-intensive kernel that consumed over 90% of the run time and had moderate amounts of communication over the interconnect."

According to Langer, 20 different functions accounted for 95% of the compute time during the pF3D run. Some of these functions perform significant amounts of memory access, so pF3D could not achieve as high a percentage of peak floating-point performance as "single-kernel" codes. A pF3D process communicates extensively with many other processes, not just with nearest neighbors.

"These characteristics of pF3D make it harder to run efficiently at very high process counts than earlier Gordon Bell winners," Langer explained. "A number of other submissions will achieve a higher teraFLOPS rate than our pF3D run. Our multiphysics simulation running efficiently on very high processor counts is a major step forward."

Progress in HEDP Code Consolidation

In connection with the ASC Integrated Codes strategy, and the associated code consolidation efforts to eliminate unnecessary duplication of capability, Sandia and Lawrence Livermore are transferring selected



The final state of a Grad-Shafranov steady state solution in 2D-XY. The color background corresponds to the magnetic pressure. The arrows represent the magnetic force on the nodes, using a new discretization. The black contour lines are gas pressure contours. You can see that the arrows are normal to the contours, and that the hydro and mag forces balance each other. quired artifacts to be collected automatically as part of the workflow, thus relieving developers of onerous documentation tasks. Better communication is achieved by centralizing information and automated collaboration between team members, which improves developer productivity and quality.

magneto-hydrodynamics (MHD) capabilities developed and implemented in Sandia's ALEGRA code into Lawrence Livermore's high energy density physics (HEDP) codes. An early success was achieved in this collaboration through implementation of a package from ALEGRA for ideal MHD modeling in the Lawrence Livermore KULL code.

The new capability allows users to initialize arbitrary magnetic fields for subsequent MHD simulations. The Intrepid package in the Sandia Trilinos library is used to reconstruct the magnetic field, which is then used to calculate magnetic stresses for the hydrodynamics package.

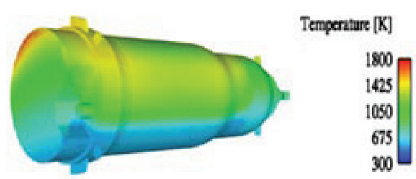
Several test problems have been created in the KULL test suite to verify each part of the code created so far, including tests for serial and parallel consistency, initialization, Intrepid tests, and some simple steady-state ideal MHD problems. The new MHD capability has been used to calculate the results of a Ryu-Jones test problem in which density, magnetic field, and pressure discontinuities generate various shock and rarefaction waves.

The KULL 2D and 3D solutions for the test problem compare well with both ALEGRA and analytic solutions. The simulations are the first 2D ideal MHD calculations ever done in KULL.

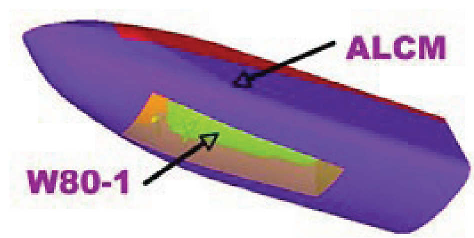
ASC Contribution Featured in W80 QMU Analysis

A quantification of margins and uncertainties (QMU) study subject to both fully engulfing and directed-flux fire scenarios was performed under the Sandia ASC Verification and Validation program for the W80-0/1. This study employed the thermal analysis capabilities of Sandia's SIERRA simulation software and the uncertainty quantification capabilities of Sandia's DAKOTA software. Sandia's Predictive Capability Maturity Model (PCMM) was used to assess the state of the physics-based computational models and the QMU analysis methods employed. The study also demonstrated new reaction rate chemistry models implemented in Sandia's SIERRA Mechanics code and used experiment data acquired from W80-0/1 thermal tests in Sandia's Radiant Heat Facility to assist with model validation.

W80-1 warhead model.



W80-1 warhead model showing predicted surface temperatures created by a hydrocarbon fuel fire.



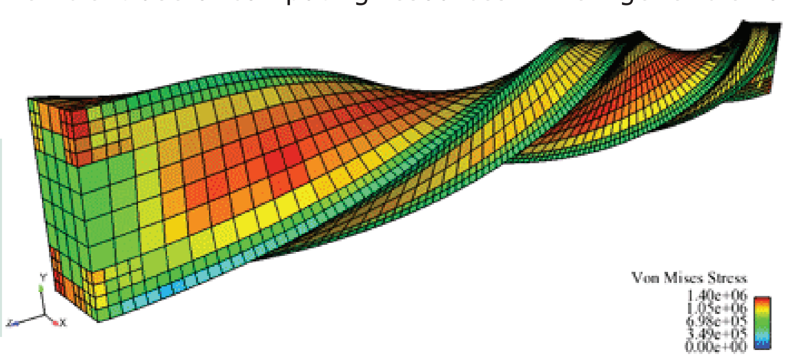
W80-1 warhead model, including Air-Launched Cruise Missile Forebody.

The results of the study were presented at the annual Sandia Stockpile Review Conference (March 2008) and provided the first abnormal thermal QMU analysis for a stockpile system under both fully engulfing and directed-flux scenarios. The thermal analysis methods and QMU methods used in this study will serve as a template for future abnormal thermal QMU analyses for other stockpile systems.

New Error Estimator Deployed in Encore

Numerical error estimation and adaptive mesh refinement are important capabilities for solution verification in modeling and simulation studies and for efficient use of computing resources. A new generic error estimator that can be used in multiple Sandia codes has been recently added to Encore—the SIERRA Mechanics toolkit for verification and adaptive mesh refinement. The estimator

Application of the new error estimator in Encore to a large rotation 3D structural torsion problem solved using the SIERRA Mechanics code Adagio. The mesh adaptivity is driven by the errors in the displacement gradients.



is based on averaging of fluxes or stresses and is independent of the physics used in the code.

This new capability is available in Encore Version 1.0 and is used by the thermal, fluids, and structural response modules in Sandia's SIERRA Mechanics code.

New V&V Capabilities Demonstrated in Neutron Generator Study

The recently developed ion beam focusing capabilities of the Aleph simulation tool were validated through comparisons to experimental data on gradients in high electrostatic fields. The project is jointly funded by the SNL ASC Verification and Validation program and Integrated Codes program, The Aleph code is being developed as the code platform for modeling the plasma source generation, as well as the acceleration and transport of the ionized plasma, in the high-voltage tube of neutron generators.

The recent validation study employed Sandia's DAKOTA toolkit to explore the sensitivity of ion beam performance to variations in electron temperature, ion temperature, and accelerating voltage. The study used Sandia's SIERRA/Encore software tool to perform comparisons of the Aleph simulation data with the experimental test data.

Sequoia: Supporting Urgent Stockpile Stewardship Computing Needs

The signing of Sequoia Critical Decision 1 (CD1) by NNSA Deputy Administrator Robert L. Smolen on March 26, 2008, allows Lawrence Livermore National Laboratory to release the Sequoia Request for Proposal (RFP) to the industry for bid. This development sets the program on a date-certain path for evaluation of RFP responses, vendor selection, contract negotiation, and acquisition of a new petascale computing resource.

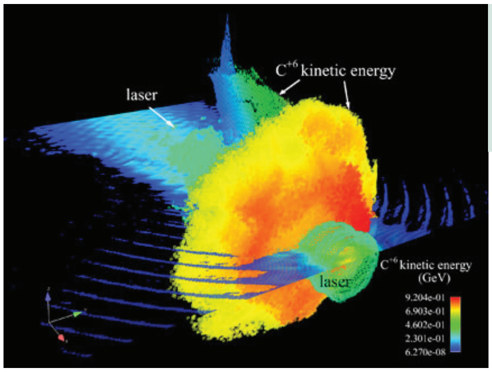
The Sequoia project will deploy an 8 to 25 petaFLOPS computer system in late 2011 or early 2012 as a national user facility for Stockpile Stewardship Program needs. In addition to this 2011 to 2012 system delivery, the vendor contract will provide a smaller but significant initial delivery (ID) computing system to be delivered in early 2009 for the code development and scaling necessary for effective use of the final petascale system. The Sequoia acquisition strategy also plans to request technology research and development (R&D) roadmaps from vendors as part of their RFP responses, with an intent that the project will fund an R&D effort for the winning vendor to address identified risks and issues for the platform build and delivery.

Both the ID and final systems will support important programmatic deliverables, including weapons certification and annual assessment, the National Boost Initiative, significant finding investigations, life extension programs, complex-transforming advanced certification campaigns, and the design of experiments at NNSA facilities, such as the National Ignition Facility and the Dual Axis Radiographic Hydrodynamic Test facility.

The ASC Roadmap (http://www.sandia.gov/NNSA/ASC/pdfs/ASC-RdMap1206r.pdf), published in 2006, provides programmatic justifications for petascale (and eventually, exascale) computing. A more recently published ASC Platform Strategy (http://www.sandia.gov/NNSA/ASC/pdfs/AscPlatform2007.pdf) document responded to these programmatic drivers with a new platforms roadmap that tasks ASC to deliver the necessary computing resources. In particular, to quantify uncertainty and address mission needs of NNSA's Stockpile Stewardship Program (SSP), the Sequoia project will provide computational resources up to 50 times more capable than current production weapons and science ASC platforms. Sequoia will bridge the gap between current terascale Purple, Red Storm, and BlueGene/L systems and exascale systems that will become available within a decade.

The New Frontier of Research: Science at the Petascale

In early June 2008, while verifying the performance of the Los Alamos National Laboratory Roadrunner supercomputer, Los Alamos and IBM researchers used three different computational codes to test the machine: VPIC, SPaSM, and PetaVision. VPIC simulates plasma physics. For example, one application of VPIC is to simulate laser plasma interactions critical to understanding inertial confinement fusion at the National Ignition Facility. SPaSM simulations provide insight into fundamental materials and physics processes. PetaVi-



A simulation of laser interaction with a carbon target using the VPIC code.

sion models the human visual system—mimicking more than one billion visual neurons and trillions of synapses. Scientists used PetaVision to reach a new computing performance record of a sustained 1.144 petaFLOPS.

Roadrunner is an advanced architecture with a very exciting future in terms of science and social exploitation of new technologies. Applications will foster scientific discovery in many fields, ranging from physical sciences to biology and medicine.

See the June 13, 2008, LANL press release "Roadrunner supercomputer puts research at a new scale" at http://www.lanl.gov/news/index.php/fuseaction/home.story/story_id/13602.

Roadrunner in Running for TOP500 and Green500 Lists

Making it onto the TOP500 list of supercomputers is a much sought-after goal. At the end of May 2008, Roadrunner posted a peak performance of 1.026 petaFLOPS running the Linpack benchmark. The test consisted of solving linear equations involving more than 2 million equations and an equal number of unknowns.

The 31st TOP500 list will be released on June 18, 2008, at the Opening Session of the 23rd Annual International Supercomputing Conference (ISC) in Dresden, Germany. "For me, breaking the petaflop/s barrier is the equivalent of a runner finally running the 100-meter race in 9.5 seconds—a level of performance everyone hopes for but proves elusive to actually achieve," said Prof. Hans Meuer, general chair of ISC and founder of the TOP500 list.

ISC will acknowledge this historic milestone with a special panel discussion "Roadrunner—the First Petaflop/s System in the World and Its Impact on Supercomputing." Dr. Andrew White (Los Alamos National Laboratory) and Dr. Don Grice (IBM) will participate in the session along with some of the most respected high-performance computing experts from North America, Asia, and Europe. Two authors of the TOP500 list will join them, Dr. Jack Dongarra (University of Tennessee) and Dr. Erich Strohmaier (Lawrence Berkeley National Laboratory).

Visit the TOP500 list at http://www.top500.org/tags/top500.

Submissions for the Green500 list are due on June 18, 2008, and runs from Roadrunner will be submitted to showcase its energy efficiency. The first Green500 list was released at Supercomputing 07, the international conference for high performance computing, networking, storage, and analysis. The list was started to raise awareness of energy efficiency for improved reliability. See the Green500 at http://www.green500.org/lists/2008/02/green500.php.

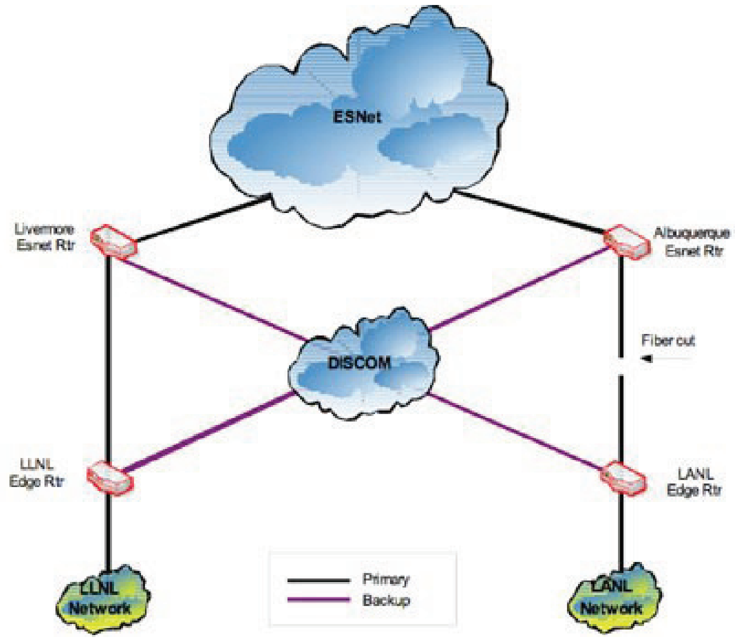
Backup Internet Path Saves Los Alamos Connection

On April 15, 2008, a cut fiber cable near Santa Fe, NM, caused a complete loss of Internet connectivity at Los Alamos National Laboratory. Fortunately, LANL network engineers were able to activate a backup path within minutes, re-routing their Internet traffic across the DISCOM WAN and back onto ESNet in Livermore. The backup connection remained active for nearly 22 hours while the fiber cut was repaired. In most circumstances, this incident would have been disastrous, but thanks to the bidirectional backup path to the Internet developed by teams at LLNL and LANL and implemented just five weeks earlier, LANL was back online within minutes.

To make this emergency response possible, network engineers from LLNL and LANL had designed and configured a backup Internet connection using the ASC-funded DISCOM network. The system was designed to protect LLNL and LANL from worst-case scenarios that could disrupt their connection to ESNet, their sole Internet service provider. One such scenario, a fiber cut between LLNL and its next-hop ESNet facility in Santa Clara or between LANL and its next-hop ESNet facility in Albuquerque was deemed unlikely, but it was projected to have a major impact if it occurred.

"We did not test anything quite as drastic as disconnecting the primary link (to simulate a cable cut)," said Robin Goldstone, associate program leader at LLNL for Networks and Convergence, who is responsible for strategic planning of its unclassified network capabilities. "We did perform a real-world validation of the connectivity in late February," she continued. "We demonstrated we could fail over to the backup link without any interruption in connectivity, perform planned maintenance, then fail back seamlessly. When the actual 'disaster' occurred, everything worked just as expected."

Without the foresight, creativity, and technical skill of the joint LLNL/LANL network engineering team, last week's outage would have caused significant impact to LANL's ability to conduct business. LLNL stands to benefit from this experience if a similar situation occurs on its end of the network.

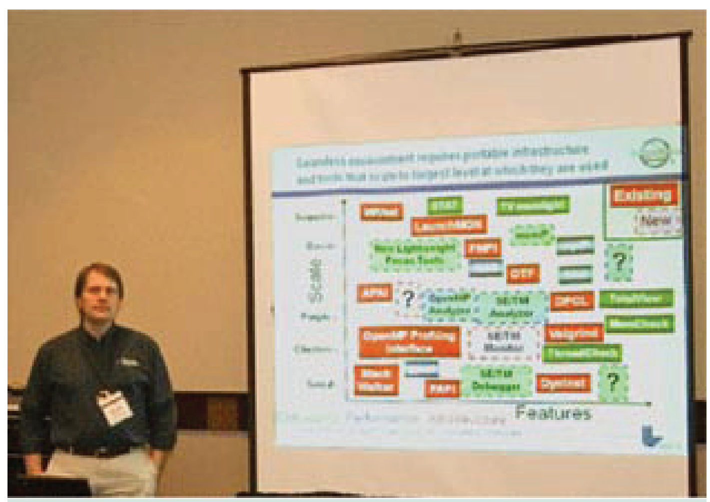


This diagram shows the location of the fiber cut (right) that disrupted LANL's Internet services on April 15.

ASC Participates in First-Ever Office of Science HPC Symposium

ASC researchers were prominently represented in the first High Performance Computer Science Week (HPCSW), organized by DOE's Office of Science in collaboration with the Krell Institute, held March 30 to April 4 in Denver, CO. The first half of the week featured a meeting of all principal investigators of the Office of Advanced Scientific Computing Research (OASCR) Computer Science projects, and the second week offered a comprehensive overview of the state of the art in HPC through one keynote, four panels, seven workshops, and two tutorials.

Researchers from the tri-lab community (LLNL, LANL, and SNL) represented a wide range of DOE/OASCR-funded projects from systems research to visualization. The program also featured an invited presentation by LLNL's Nathan Barton on the Cooperative Parallelism (COOP) framework developed at LLNL to support large-scale coupled simulations.

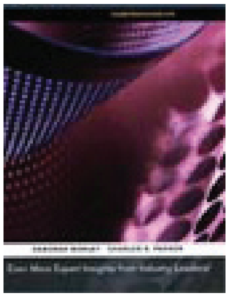


Bronis de Supinski (LLNL) presents his invited talk on Autotuning.

The HPCSW program in the second half of the week contained an international workshop on interoperable tool infrastructures with participation from several research groups in the U.S. and Germany. Organized by Martin Schulz and Bronis de Supinski (LLNL), David Montoya (LANL), and Jim Galarowicz (Krell Institute), it provided the stage for extensive discussions on how to build reusable software components that can be used across individual tools and how to scale them to future machines.

The Open|SpeedShop team represented by Schulz, Montoya, and Galarowicz presented a tutorial focusing on performance analysis using the ASC toolset Open|SpeedShop, and de Supinski gave an invited presentation at a workshop on Autotuning organized by Mary Hall (Information Sciences Institute/USC).

BlueGene/L Referenced As State-of-the-Art in College Textbook



BlueGene/L is referenced as an example of state-of-the-art supercomputing in a newly published college textbook, Understanding Computers Today and Tomorrow. The textbook, now in its 12th edition, is published by Cenage Learning as part of its Course Technology series. BlueGene/L is referenced with photos in a section on supercomputers and supercomputing clusters and again in a section on massively parallel processing. The text is edited by Deborah Morley and Charles S. Parker and sells in hard copy for about $85.

ASC Salutes

Martin Heinstein, a Distinguished Member of the Technical Staff in the Engineering Sciences Center at Sandia, leads the computational solid mechanics portion of Sandia's SIERRA Mechanics development effort under ASC's Integrated Codes/Engineering Codes program element. In the four years that Martin has served in this role, SIERRA Mechanics has moved from a loosely connected set of mechanics modules to a more tightly consolidated code system, which is reliable and robust, with dramatic performance increases and unique mechanics capabilities for Sandia's diverse set of solid/structural mechanics applications. These capabilities have also been extended to applications across the nuclear weapons complex. With his ability to create innovative solutions to mechanics problems, Martin has been directly responsible for the successful development of many of these unique capabilities and for guiding the work of others in developing additional capabilities.

Some of his contributions to SIERRA Mechanics include multi-level algorithms for solving large, nonlinear quasi-statics problems with iterative solution methods; efficient and robust contact algorithms for explicit dynamics and quasi-statics; and multi-length-scale algorithms for fracture and failure. Additionally, Martin has been a key player in the development of a nodal-based tetrahedral element (with computational properties comparable to single-point integrated hexahedral elements), which, when applied with remeshing algorithms, allows successful application of Lagrangian methods to problems involving extremely large deformations. He has also led work on a time-stepping algorithm for explicit dynamics applications, which can produce speed-ups of 20X or more for some problems.

Martin received his PhD in Aerospace/Engineering Mechanics from Purdue University in 1989 and joined Sandia in early 1992 as a Postdoctoral Fellow. He became a technical staff member at Sandia in late 1992. In addition to his contributions to the ASC Program, Martin has been a key participant in Sandia's highly successful CRADA partnership with the Goodyear Tire and Rubber Company. Martin's computational algorithms provided Goodyear with a unique computational mechanics capability that led to a revolutionary change from a test-based to a computational-based design culture at Goodyear. Martin, along with his Goodyear and Sandia colleagues, received an R&D 100 Award for designing and producing innovative new tires in record times through the use of this computational simulation capability. Martin was also part of the SNL team that developed the first scalable parallel contact algorithm, which has received numerous awards in the computational mechanics community.

Under Martin's leadership, the SIERRA Mechanics code has been used for many nuclear weapons applications, including extensive use in recent design and qualification studies for the W76-1. Issues addressed include determining margins and uncertainties for weld attachments of the firing set exclusion region and resolving a major shock-unlock issue with the intent strong link. In another application, SIERRA Mechanics was used to investigate safety scenarios for the SafeGuard Trailer (SGT) used for nuclear weapons transport. Failure capabilities in SIERRA Mechanics are being used to provide more accurate solutions for crash scenarios.

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Developed and maintained by Sandia National Laboratories for NA.114

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy's National Nuclear Security Administration
under contract DE-AC04-94AL85000.

SAND 2008-4454 W